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CDAC Activity Report

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Activity Summary

We have received CDAC allotments of beam time at HPCAT that were used to carryout investigations that included angle-dispersive x-ray diffraction of beryllium at high pressures and inelastic x-ray scattering (x-ray Raman) of high pressure phases of water. These CDAC beam time allotments have permitted us to broaden and supplement the scope of our research. The beam time has also been used in experiments that had graduate student participants (Z Jenei and A Lazicki) and thus the experiments also incorporated a component of training and education.

Water (H_2O) is a major constituent of terrestrial systems, and furthering our understanding of this ubiquitous system and hydrogen bonding structures impacts a broad range of systems; including geophysics, life sciences, the environment and technology development. Our inelastic x-ray scattering studies (x-ray Raman spectroscopy) of high-pressure phases of water and ice are aimed at addressing controversies regarding the high-pressure structure of water. Using the inelastic x-ray scattering system at HPCAT we have measured x-ray Raman spectra of water at 1 and 17 GPa. X-Ray Raman is a relatively new technique that provides data that is equivalent to x-ray absorption, but utilizes a hard x-ray to avoid short absorption lengths and surface effects to achieve a truly bulk measurement. These are extremely challenging measurements that rely on optimized experimental systems and the brilliance of a 3rd generation synchrotron source. The figure below shows our specially designed diamond and the general operation of the x-ray scattering system.

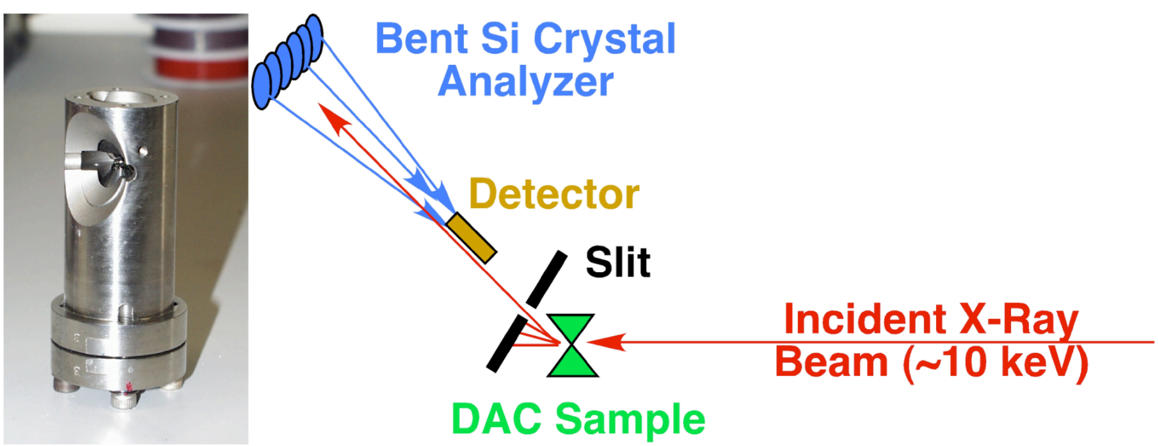

Figure. X-ray Raman cell and schematic. Left - image of LLNL SAX cell, with large aperture for collecting inelastically scattered photons. Right - schematic of system.

Though our work is at a preliminary stage, we have measured x-ray Raman spectra of water (H_2O) in phases VI and VII. These spectra are shown in figure 2. Using sophisticated modeling techniques developed by our collaborators, U. Bergmann and A

Nillson, these spectra can be used to test and validate different models of the local structure and bonding of water molecules. We plan to continue this work extending it to higher pressures and temperatures.

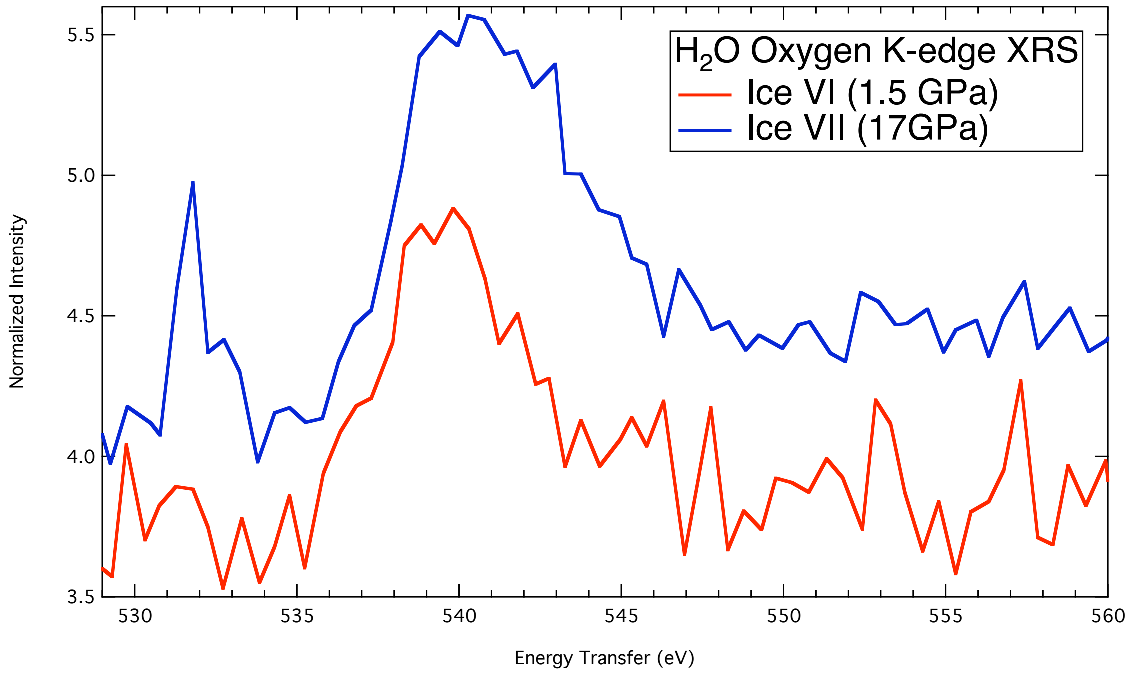

Figure. X-ray Raman spectra of H_20 in two of its room temperature high pressure phases.

We have also used CDAC beam time allotments to study the high-pressure behavior and equation of state of beryllium. Beryllium is an important material for the nuclear power industry and a broad range of advanced technologies (aerospace, alloys, x-ray windows). Beryllium has been described as an anomalous metal because of its unusual physical properties, but it is also one of the simplest metals with only four electrons per atom. Thus studies of beryllium are also of basic scientific interest as a model system for developing predictive theoretical models. We have studied the crystal structure and determined the equation-of-state of beryllium up to pressures approaching 200 GPa. These works are presented in a manuscript that has been accepted for publication in Physical Review B.

Acknowledgements

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CDAC-Related Presentations
High Pressure Beryllium: Static & Elastic Properties, Joint 20th AIRAPT - 43rd EHPRG International Conference on High Pressure Science and Technology, Karlsruhe, Germany, 2005

CDAC-Related Publications
X-Ray Diffraction and Raman Studies of Beryllium: Static and Elastic Properties at High Pressures, Physical Review B, accepted for publication